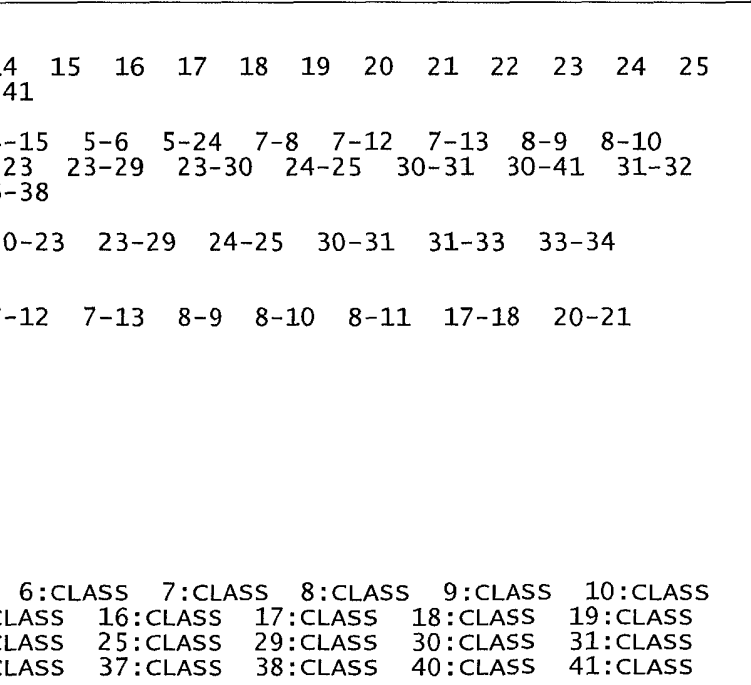


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2 ANSWERS

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TOTAL

ENTRY

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FULL ESTIMATED COST

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148.36

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FILE COVERS 1907 - 25 Sep 2003 VOL 139 ISS 13

FILE LAST UPDATED: 24 Sep 2003 (20030924/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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18916699 PY<1999

L4 0 L3 AND PY<1999

=> l3 and py<2000

19719652 PY<2000

L5 1 L3 AND PY<2000

=> d bib

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1999:795834 CAPLUS

DN 132:36034

TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease

IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella

PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy

SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
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 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG

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 AU 9942798 A1 19991230 AU 1999-42798 19990609 <--
 AU 754773 B2 20021121
 EP 1084137 A1 20010321 EP 1999-955475 19990609

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE

PRAI GB 1998-12523 A 19980610
 WO 1999-GB1824 W 19990609

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 19719652 PY<2000
 L10 1 L9 AND PY<2000
 => d bib 1

L10 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1999:795834 CAPLUS

DN 132:36034

TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella

PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy

SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
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	WO 1999-GB1824	W	19990609			

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> l9 d bib 2

MISSING OPERATOR L9 D BIB

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

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L9 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2002:116981 CAPLUS

DN 137:149812

TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease

AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.

CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy

SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704

CODEN: BMCLE8; ISSN: 0960-894X

PB Elsevier Science Ltd.

DT Journal

LA English

RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L9 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2003 ACS on STN

AN 2000:68910 CAPLUS

DN 132:245829

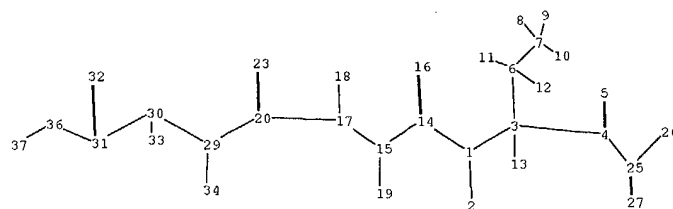
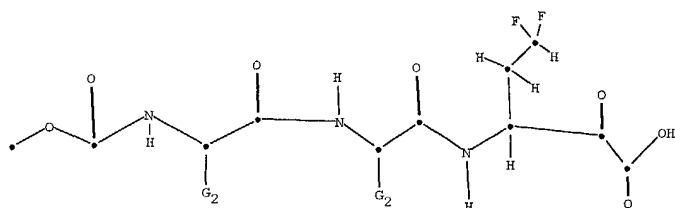
TI .alpha.-Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C Virus NS3 Protease

AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella; Fattori, Daniela; De Francesco, Raffaele; Matassa, Victor G.; Steinkuehler, Christian

CS Departments of Biochemistry Medicinal Chemistry and Computational Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, Pomezia, 00040, Italy

SO Biochemistry (2000), 39(7), 1849-1861

CODEN: BICHAW; ISSN: 0006-2960



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31-36 36-37

exact/norm bonds :

1-3 1-14 4-5 14-16 15-17 15-19 17-20 20-23 29-30 29-34 30-31 31-32 31-36
36-37

exact bonds :

1-2 3-13 3-6 3-4 4-25 6-7 6-11 6-12 7-8 7-9 7-10 14-15 17-18 20-29 30-33

normalized bonds :

25-26 25-27

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

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11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
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PB American Chemical Society
DT Journal
LA English
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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L18 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:795834 CAPLUS
DN 132:36034
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
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 CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
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 AU 9942798 A1 19991230 AU 1999-42798 19990609
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 EP 1084137 A1 20010321 EP 1999-955475 19990609
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 PRAI GB 1998-12523 A 19980610
 WO 1999-GB1824 W 19990609
 RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

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 L24 1 L23 AND PY<2000

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L24 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1999:795834 CAPLUS
 DN 132:36034
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma,
 Marco; Marchetti, Antonella
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
 SO PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE
PRAI GB 1998-12523 A 19980610
WO 1999-GB1824 W 19990609
RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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SEARCH TIME: 00.00.01

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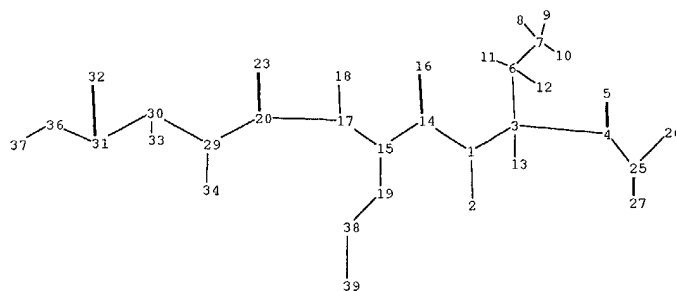
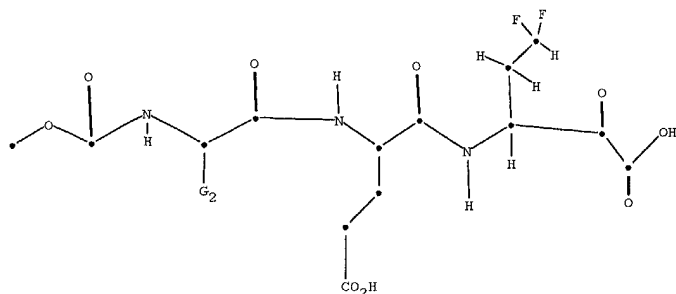
L4 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:795834 CAPLUS
DN 132:36034
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma,
Marco; Marchetti, Antonella
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti s.p.A., Italy
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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AU 754773	B2	20021121		
EP 1084137	A1	20010321	EP 1999-955475	19990609
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AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
PRAI GB 1998-12523	A	19980610		
WO 1999-GB1824	W	19990609		
RE.CNT 3				
THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD				
ALL CITATIONS AVAILABLE IN THE RE FORMAT				

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exact/norm bonds :

1-3 1-14 4-5 14-16 15-17 17-20 20-23 29-30 29-34 30-31 31-32 31-36 36-37

exact bonds :

1-2 3-13 3-6 3-4 4-25 6-7 6-11 6-12 7-8 7-9 7-10 14-15 15-19 17-18 19-38
20-29 30-33 38-39

normalized bonds :

25-26 25-27

G1:H,CH₃,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH₃,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

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L3 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN

AN 1999:795834 CAPLUS

DN 132:36034

TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease

IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella

PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti s.p.A., Italy

SO PCT Int. Appl., 121 pp.

CODEN: PIXXD2

DT Patent

LA English

FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
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	AU 9942798	A1	19991230	AU 1999-42798	19990609
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	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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100.0% PROCESSED 291 ITERATIONS
SEARCH TIME: 00.00.01

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=> d bib

L5 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1999:795834 CAPLUS
 DN 132:36034
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
 SO PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609 <--
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	AU 9942798	A1	19991230	AU 1999-42798	19990609 <--
	AU 754773	B2	20021121		
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PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		
RE.CNT	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT			

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L6 STRUCTURE UPLOADED

=> 16 sss full

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Substance data SEARCH and crossover from CAS REGISTRY in progress...
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100.0% PROCESSED 473 ITERATIONS
SEARCH TIME: 00.00.01

24 ANSWERS

L7 24 SEA SSS FUL L6

L8 6 L7

=> 18 and py<2000
19719654 PY<2000

L9 1 L8 AND PY<2000

=> d bib

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1999:795834 CAPLUS
 DN 132:36034
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
 SO PCT Int. Appl., 121 pp.
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DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609	<--
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
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	EP 1084137	A1	20010321	EP 1999-955475	19990609	
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
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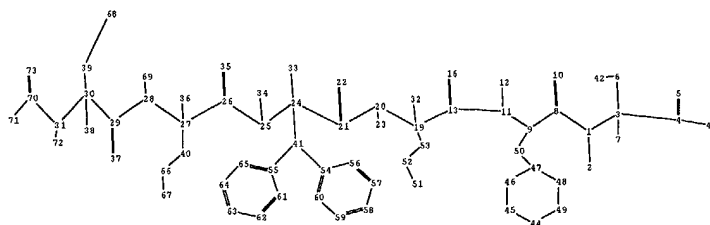
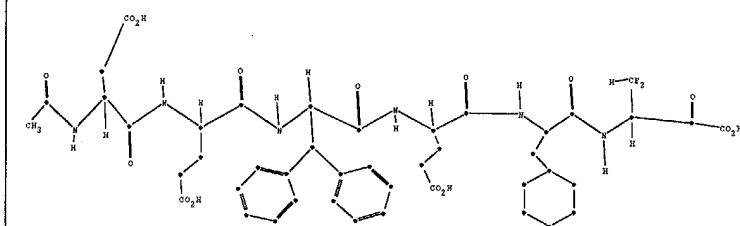
=> d 13 ab 1-5

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AB N-Terminal truncation of the hexapeptide ketoacid MeCO-Asp-Glu-NHCH(CHPh2)CO-Glu-NHCH(CH2c-C6H11)CONHCH(CH2CHF2)CO2H (all-L stereochem.) (c-C6H11= cyclohexyl) gave rise to potent tripeptide inhibitors of the hepatitis C virus NS3 protease/NS4A cofactor complex. Optimization of these tripeptides led to ketoacid BOC-NHCH(c-C5H9)CO-Leu-NHCH(CH2CHF2)COCO2H (all-L stereochem.) (BOC = tert-butoxycarbonyl, c-C5H9 = cyclopentyl) with an IC50 of 0.38 .mu.M. The SAR of these tripeptides is discussed in the light of the recently published crystal structures of a ternary tripeptide/NS3/NS4A complexes.

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AB The difluoromethyl group was designed by computational chem. methods as a mimetic of the canonical P1 cysteine thiol for inhibitors of the hepatitis C virus NS3 protease. This modification led to the development of competitive, non-covalent inhibitor AcAspGlu-NHCH(CHPh2)CO-Glu-NHCH(CH2C6H11)CONHCH(CH2CHF2)R (I, R = CHO) Ki 30 nM and reversible covalent inhibitors (I, R = CO2H) Ki 0.5 nM; and (I, R = COCO2H) Ki* 10 pM.

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AB A serine protease domain contained within the viral NS3 protein is a key player in the maturational processing of the hepatitis C virus polyprotein and a prime target for the development of antiviral drugs. In the present work, we describe a dansylated hexapeptide inhibitor of this enzyme. Active site occupancy by this compd. could be monitored following fluorescence resonance energy transfer between the dansyl fluorophore and protein tryptophan residues and could be used to (1) unambiguously assess active site binding of NS3 protease inhibitors, (2) directly det. equil. and pre-steady-state parameters of enzyme-inhibitor complex formation, and (3) dissect, using site-directed mutagenesis, the contribution of single residues of NS3 to inhibitor binding in direct binding assays. The assay was also used to characterize the inhibition of the NS3 protease by its cleavage products. We show that enzyme-product inhibitor complex formation depends on the presence of an NS4A cofactor peptide. Equil. and pre-steady-state data support an ordered mechanism of ternary (enzyme-inhibitor-cofactor) complex formation, requiring cofactor complexation prior to inhibitor binding.

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AB The replication of the hepatitis C virus (HCV), an important human pathogen, crucially depends on the proteolytic maturation of a large viral polyprotein precursor. The viral nonstructural protein 3 (NS3) harbors a serine protease domain that plays a pivotal role in this process, being responsible for four out of the five cleavage events that occur in the nonstructural region of the HCV polyprotein. We here show that hexapeptide, tetrapeptide, and tripeptide .alpha.-ketoacids are potent, slow binding inhibitors of this enzyme. Their mechanism of inhibition



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 16 19 20 21 22 23 24 25 26 27 28 29
30 31 32 33 34 35 36 37 38 39 40 41 42 43 50 51 52 53 66 67 68 69
70 71 72 73

ring nodes :

44 45 46 47 48 49 54 55 56 57 58 59 60 61 62 63 64 65

chain bonds :

1-2 1-3 1-8 3-7 3-6 3-4 4-5 4-43 6-42 8-9 8-10 9-11 9-50 11-12 11-13 13-16
13-19 19-20 19-32 19-53 20-21 20-23 21-22 21-24 24-25 24-33 24-41 25-26 25-34
26-27 26-35 27-28 27-36 27-40 28-29 28-69 29-30 29-37 30-31 30-38 30-39 31-70
31-72 39-68 40-66 41-54 41-55 47-50 51-52 52-53 66-67 70-71 70-73

ring bonds :

44-45 44-49 45-46 46-47 47-48 48-49 54-60 54-56 55-65 55-61 56-57 57-58 58-59
59-60 61-62 62-63 63-64 64-65

exact/norm bonds :

1-3 1-8 4-5 8-10 9-11 11-13 13-16 19-20 20-21 21-22 24-25 25-26 26-35 27-28
28-29 29-37 30-31 31-70 44-45 44-49 45-46 46-47 47-48 48-49 70-73

exact bonds :

1-2 3-7 3-6 3-4 4-43 6-42 8-9 9-50 11-12 13-19 19-32 19-53 20-23 21-24
24-33 24-41 25-34 26-27 27-36 27-40 28-69 29-30 30-38 30-39 31-72 39-68 40-66
41-54 41-55 47-50 51-52 52-53 66-67 70-71

normalized bonds :

54-60 54-56 55-65 55-61 56-57 57-58 58-59 59-60 61-62 62-63 63-64 64-65

G1:H,CH₃,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH₃,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 16:CLASS 19:CLASS 20:CLASS 21:CLASS 22:CLASS 23:CLASS
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51:CLASS 52:CLASS 53:CLASS 54:Atom 55:Atom 56:Atom 57:Atom 58:Atom 59:Atom
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69:CLASS 70:CLASS 71:CLASS 72:CLASS 73:CLASS

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SEARCH TIME: 00.00.01

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L2 0 SEA SSS FUL L1

=> l1 exa full

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100.0% PROCESSED 5 ITERATIONS

SEARCH TIME: 00.00.01

0 ANSWERS

L3 0 SEA EXA FUL L1

=>

Uploading coreitalianpeptide.str

L4 STRUCTURE UPLOADED

=> l4 exa full

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FULL SCREEN SEARCH COMPLETED - 5 TO ITERATE

100.0% PROCESSED 5 ITERATIONS

SEARCH TIME: 00.00.01

0 ANSWERS

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=> l4 sss full

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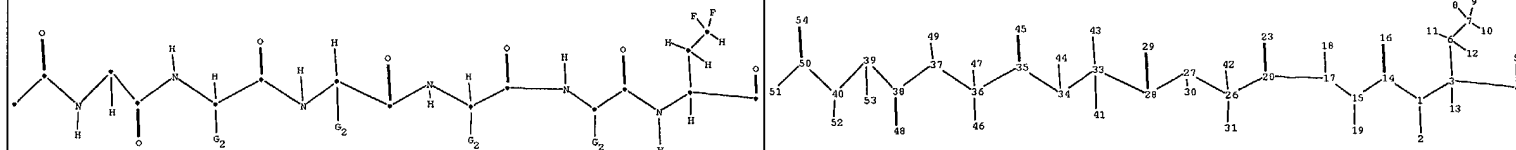
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100.0% PROCESSED 15 ITERATIONS

SEARCH TIME: 00.00.01

0 ANSWERS

L6 0 SEA SSS FUL L4



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 23 26 27 28 29
30 31 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52
53 54

chain bonds :

1-2 1-3 1-14 3-13 3-6 3-4 4-5 6-7 6-11 6-12 7-8 7-9 7-10 14-15 14-16 15-17
15-19 17-18 17-20 20-23 20-26 26-27 26-31 26-42 27-28 27-30 28-29 28-33 33-34
33-41 33-43 34-35 34-44 35-36 35-45 36-37 36-46 36-47 37-38 37-49 38-39 38-48
39-40 39-53 40-50 40-52 50-51 50-54

exact/norm bonds :

1-3 1-14 4-5 14-16 15-17 15-19 17-20 20-23 26-27 26-31 27-28 28-29 33-34
33-41 34-35 35-45 36-37 36-46 37-38 38-48 39-40 40-50 50-54

exact bonds :

1-2 3-13 3-6 3-4 6-7 6-11 6-12 7-8 7-9 7-10 14-15 17-18 20-26 26-42 27-30
28-33 33-43 34-44 35-36 36-47 37-49 38-39 39-53 40-52 50-51

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

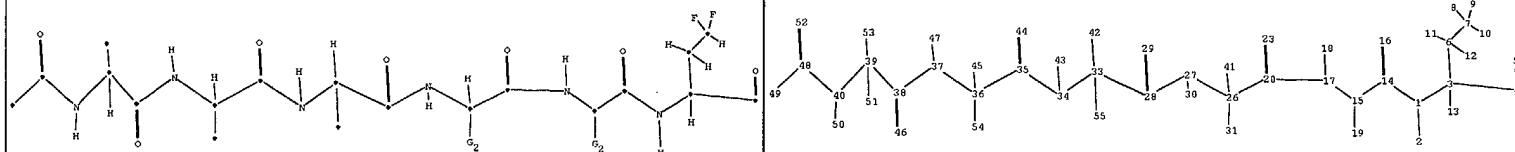
G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 23:CLASS 26:CLASS 27:CLASS 28:CLASS 29:CLASS 30:CLASS 31:CLASS 33:CLASS
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52:CLASS 53:CLASS 54:CLASS



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 23 26 27 28 29
 30 31 33 34 35 36 37 38 39 40 41 42 43 44 45 46 47 48 49 50 51 52
 53 54 55

chain bonds :

1-2 1-3 1-14 3-13 3-6 3-4 4-5 6-7 6-11 6-12 7-8 7-9 7-10 14-15 14-16 15-17
 15-19 17-18 17-20 20-23 20-26 26-27 26-31 26-41 27-28 27-30 28-29 28-33 33-34
 33-42 33-55 34-35 34-43 35-36 35-44 36-37 36-45 36-54 37-38 37-47 38-39 38-46
 39-40 39-51 39-53 40-48 40-50 48-49 48-52

exact/norm bonds :

1-3 1-14 4-5 14-16 15-17 15-19 17-20 20-23 26-27 26-31 27-28 28-29 33-34
 34-35 35-44 36-37 37-38 38-46 39-40 40-48 48-52

exact bonds :

1-2 3-13 3-6 3-4 6-7 6-11 6-12 7-8 7-9 7-10 14-15 17-18 20-26 26-41 27-30
 28-33 33-42 33-55 34-43 35-36 36-45 36-54 37-47 38-39 39-51 39-53 40-50 48-49

G1:H,CH3,n-Bu,i-Bu,s-Bu,t-Bu,Ph,Cb,Ak

G2:Cb,Ak

G3:Cy,Ak,CH3,n-Bu,i-Bu,s-Bu,t-Bu

G4:Hy,H

Match level :

1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
 11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
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 43:CLASS 44:CLASS 45:CLASS 46:CLASS 47:CLASS 48:CLASS 49:CLASS 50:CLASS 51:CLASS
 52:CLASS 53:CLASS 54:CLASS 55:CLASS

involves the rapid formation of a noncovalent collision complex in a diffusion-limited, electrostatically driven assocn. reaction followed by a slow isomerization step resulting in a very tight complex. pH dependence expts. point to the protonated catalytic His 57 as an important determinant for formation of the collision complex. K_i values of the collision complexes vary between 3 nM and 18.5 μ M and largely depend on contacts made by the peptide moiety of the inhibitors. Site-directed mutagenesis indicates that Lys 136 selectively participates in stabilization of the tight complex but not of the collision complex. A significant solvent isotope effect on the isomerization rate const. is suggestive of a chem. step being rate limiting for tight complex formation. The potency of these compds. is dominated by their slow dissocn. rate consts., leading to complex half-lives of 11-48 h and overall K_i values between 10 pM and 67 nM. The rate consts. describing the formation and the dissocn. of the tight complex are relatively independent of the peptide moiety and appear to predominantly reflect the intrinsic chem. reactivity of the ketoacid function.

L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
 AB Fluorinated oligopeptides Y-B-A-X or Y-B-A'-X' [A is an amino acid residue NHCH(CH₂CHF₂)(CH₂)_mCO and A' is NHCHR₁(CH₂)_mCO (m = 0, 1; R₁ is a fluorine-substituted hydrocarbyl side chain); B is a naturally or non-naturally occurring amino acid residue NHCHR₂CO (R₂ is a nonpolar or polar but uncharged side chain or is a side chain contg. an acidic functionality); X = CO₂R₈, H, OR₈, CF₃, CONR₉R₁₀, NHSO₂R₂₅, or certain 5-membered heterocyclic groups (R₈, R₉, R₁₀, R₂₅ = H, alkyl, alkenyl, aryl, aralkyl); X' = NHSO₂N₂₅; Y = Z-F-E-D-C (C is a natural or non-natural amino acid residue having non-polar, polar but uncharged, or acidic side chains; D, E, and F may be absent or represent a natural or non-natural amino acid; Z is absent, H, or R₇CO which forms an amide, urethane, or urea linkage with the nitrogen atom to which it is attached) or R₁₃CO (R₁₃ is an aliph. or arom. group contg. 1-25 carbon atoms, 0-5 oxygen atoms, 0-3 nitrogen atoms, 0-2 sulfur atoms, and up to 9 other heteroatoms)] were prepd. as inhibitors of hepatitis C virus NS3 protease. Thus, Ac-Asp-Glu-Met-Glu-NHCH(CH₂CHF₂)CO₂H-(s), prepd. by coupling of (S)-tert-Bu 2-amino-4,4-difluorobutanoate hydrochloride with protected pentapeptide, showed IC₅₀ for inhibition of NS3 protease.

=> d bib 1-5

L9 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1999:795834 CAPLUS
 DN 132:36034
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
 SO PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE	
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609	<--
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	AU 9942798	A1	19991230	AU 1999-42798	19990609	<--
	AU 754773	B2	20021121			
	EP 1084137	A1	20010321	EP 1999-955475	19990609	
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
PRAI	GB 1998-12523	A	19980610			
	WO 1999-GB1824	W	19990609			
RE.CNT	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT				

=> d 13 bib 1-5

L3 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:116982 CAPLUS
DN 137:47425
TI Evolution, synthesis and SAR of tripeptide .alpha.-ketoacid inhibitors of the hepatitis C virus NS3/NS4A serine protease
AU Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte, Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 137:47425
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:116981 CAPLUS
DN 137:149812
TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of HCV NS3 protease
AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin; Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura, Sergio; De Francesco, Raffaele; Matassa, Victor G.
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:352482 CAPLUS
DN 133:189820
TI Probing the active site of the hepatitis C virus serine protease by fluorescence resonance energy transfer
AU Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele; Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor G.; De Francesco, Raffaele; Steinkuhler, Christian
CS Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040, Italy
SO Journal of Biological Chemistry (2000), 275(20), 15106-15113
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:68910 CAPLUS
DN 132:245829
TI .alpha.-Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C Virus NS3 Protease
AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Biasiol, Gabriella; Fattori, Daniela; De Francesco, Raffaele; Matassa, Victor G.; Steinkuehler, Christian
CS Departments of Biochemistry Medicinal Chemistry and Computational Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P. Angeletti, Pomezia, 00040, Italy
SO Biochemistry (2000), 39(7), 1849-1861
CODEN: BICHAW; ISSN: 0006-2960
PB American Chemical Society
DT Journal
LA English
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1999:795834 CAPLUS
DN 132:36034

TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
SO PCT Int. Appl., 121 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
	W:	AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
	RW:	GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG			
	CA 2330247	AA	19991216	CA 1999-2330247	19990609
	AU 9942798	A1	19991230	AU 1999-42798	19990609
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
	R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE			
PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		
RE.CNT	3	THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT			

L1 STRUCTURE UPLOADED

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FULL SEARCH INITIATED 09:25:45 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 445 TO ITERATE

100.0% PROCESSED 445 ITERATIONS 24 ANSWERS
SEARCH TIME: 00.00.01

L2 24 SEA SSS FUL L1

=> l2
L3 6 L2

=> D bib 1-6

L3 ANSWER 1 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:777963 CAPLUS
DN 137:295254
TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
IN Colarusso, Stefania; Gardelli, Cristina; Gerlach, Benjamin; Harper, Steven; Koch, Uwe; Matassa, Victor Giulio; Muraglia, Ester; Narjes, Frank; Ontoria, Ontoria Jesus Maria; Petrocchi, Alessia; Ponzi, Simona; Stansfield, Ian; Summa, Vincenzo
PA Istituto di Ricerche di Biologia Molecolare P. Angeletti Spa, Italy; et al.
SO PCT Int. Appl., 151 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2002079234	A1	20021010	WO 2002-EP3435	20020326
	W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM			
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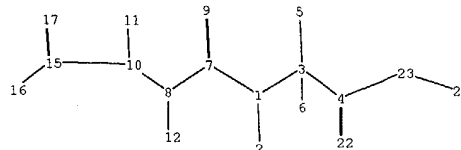
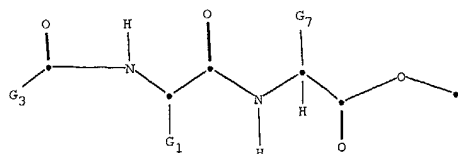
BF, BJ, CF, CG, CH, CM, GA, GN, GQ, GW, ML, MR, NE, NN, TD, TG
PRAI GB 2001-7924 A 20010329
OS MARPAT 137:295254
RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:116982 CAPLUS
DN 137:47425
TI Evolution, synthesis and SAR of tripeptide .alpha.-ketoacid inhibitors of
the hepatitis C virus NS3/NS4A serine protease
AU Colarusso, Stefania; Gerlach, Benjamin; Koch, Uwe; Muraglia, Ester; Conte,
Immacolata; Stansfield, Ian; Matassa, Victor G.; Narjes, Frank
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 705-708
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 137:47425
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2002:116981 CAPLUS
DN 137:149812
TI A designed P1 cysteine mimetic for covalent and non-covalent inhibitors of
HCV NS3 protease
AU Narjes, Frank; Koehler, Konrad F.; Koch, Uwe; Gerlach, Benjamin;
Colarusso, Stefania; Steinkuhler, Christian; Brunetti, Mirko; Altamura,
Sergio; De Francesco, Raffaele; Matassa, Victor G.
CS Department of Chemistry, MRL Rome, IRBM, Rome, Pomezia, 00040, Italy
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(4), 701-704
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
RE.CNT 27 THERE ARE 27 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:352482 CAPLUS
DN 133:189820
TI Probing the active site of the hepatitis C virus serine protease by
fluorescence resonance energy transfer
AU Fattori, Daniela; Urbani, Andrea; Brunetti, Mirko; Ingenito, Raffaele;
Pessi, Antonello; Prendergast, Kristine; Narjes, Frank; Matassa, Victor
G.; De Francesco, Raffaele; Steinkuhler, Christian
CS Istituto di Ricerche di Biologia Molecolare "P. Angeletti", Rome, 00040,
Italy
SO Journal of Biological Chemistry (2000), 275(20), 15106-15113
CODEN: JBCHA3; ISSN: 0021-9258
PB American Society for Biochemistry and Molecular Biology
DT Journal
LA English
RE.CNT 42 THERE ARE 42 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
AN 2000:68910 CAPLUS
DN 132:245829
TI .alpha.-Ketoacids Are Potent Slow Binding Inhibitors of the Hepatitis C
Virus NS3 Protease
AU Narjes, Frank; Brunetti, Mirko; Colarusso, Stefania; Gerlach, Benjamin;
Koch, Uwe; Biasiol, Gabriella; Fattori, Daniela; De Francesco, Raffaele;
Matassa, Victor G.; Steinkuehler, Christian
CS Departments of Biochemistry Medicinal Chemistry and Computational
Chemistry, Istituto di Ricerche di Biologia Molecolare (IRBM) P.
Angeletti, Pomezia, 00040, Italy
SO Biochemistry (2000), 39(7), 1849-1861
CODEN: BICAW; ISSN: 0006-2960
PB American Chemical Society
DT Journal
LA English
RE.CNT 58 THERE ARE 58 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT



chain nodes :

1 2 3 4 5 6 7 8 9 10 11 12 15 16 17 22 23 24

chain bonds :

1-2 1-3 1-7 3-4 3-5 3-6 4-22 4-23 7-8 7-9 8-10 8-12 10-11 10-15 15-17
15-16 23-24

exact/norm bonds :

1-3 1-7 3-5 4-22 4-23 7-9 8-10 8-12 10-15 15-17 15-16 23-24

exact bonds :

1-2 3-4 3-6 7-8 10-11

G1: Ak, CH3

G2: H, CF3, OH

G3: Cb, Ak

G4: C, N

G5: O, S, NH, N

G6: H, Cb, Ak

G7: CF2, CF3, F

Match level :

1: CLASS 2: CLASS 3: CLASS 4: CLASS 5: CLASS 6: CLASS 7: CLASS 8: CLASS 9: CLASS 10: CLASS
11: CLASS 12: CLASS 15: CLASS 16: CLASS 17: CLASS 22: CLASS 23: CLASS 24: CLASS

L3 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
 AN 1999:795834 CAPLUS
 DN 132:36034
 TI Preparation of peptide inhibitors of hepatitis C virus NS3 protease
 IN Matassa, Victor; Narjes, Frank; Koehler, Konrad; Ontoria, Jesus; Poma, Marco; Marchetti, Antonella
 PA Istituto Di Ricerche Di Biologia Molecolare P Angeletti S.p.A., Italy
 SO PCT Int. Appl., 121 pp.
 CODEN: PIXXD2
 DT Patent
 LA English
 FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9964442	A1	19991216	WO 1999-GB1824	19990609
	W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2330247	AA	19991216	CA 1999-2330247	19990609
	AU 9942798	A1	19991230	AU 1999-42798	19990609
	AU 754773	B2	20021121		
	EP 1084137	A1	20010321	EP 1999-955475	19990609
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE				
PRAI	GB 1998-12523	A	19980610		
	WO 1999-GB1824	W	19990609		

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

Uploading fluorinesub.str

L1 STRUCTURE UPLOADED

=> l1 sss full
 FULL SEARCH INITIATED 09:54:20 FILE 'REGISTRY'
 FULL SCREEN SEARCH COMPLETED - 137400 TO ITERATE

100.0% PROCESSED 137400 ITERATIONS 33156 ANSWERS
 SEARCH TIME: 00.00.06

L2 33156 SEA SSS FUL L1

=> file caplus		
COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	148.15	148.36

FILE 'CAPLUS' ENTERED AT 09:54:38 ON 26 SEP 2003
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FILE COVERS 1907 - 26 Sep 2003 VOL 139 ISS 14
 FILE LAST UPDATED: 25 Sep 2003 (20030925/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L3      8558 L2

=> 13 and py<2000
      19719654 PY<2000
L4      7788 L3 AND PY<2000

=> 13 and py<1999
      18916701 PY<1999
L5      7538 L3 AND PY<1999

=> d hitstr 1

L5  ANSWER 1 OF 7538  CAPLUS  COPYRIGHT 2003 ACS on STN
IT   ***145643-18-1***      ***175071-81-5***
      RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
          (topical gels contg. N-[N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-
          1-.alpha.-aspartyl]-L-phenylalanines)
RN   145643-18-1  CAPLUS
CN   L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-
      aspartyl-, dimethyl ester (9CI)  (CA INDEX NAME)
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Absolute stereochemistry.

/ structure 1 in file .gra /

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RN   175071-81-5  CAPLUS
CN   L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-
      aspartyl-, diethyl ester (9CI)  (CA INDEX NAME)
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Absolute stereochemistry.

/ structure 2 in file .gra /

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=> d hitstr 2
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L5  ANSWER 2 OF 7538  CAPLUS  COPYRIGHT 2003 ACS on STN
IT   ***149231-77-6***
      RL: RCT (Reactant); RACT (Reactant or reagent)
          (prepn. of chromophore-contg. peptides for use in detg.
          interleukin-1.beta. convertase activity)
RN   149231-77-6  CAPLUS
CN   L-Alanine, N-acetyl-L-tyrosyl-L-valyl-, phenylmethyl ester (9CI)  (CA
      INDEX NAME)
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Absolute stereochemistry.

/ structure 3 in file .gra /

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L1      STRUCTURE UPLOADED
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=> l1 sss full
FULL SEARCH INITIATED 10:01:21 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 144804 TO ITERATE
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100.0% PROCESSED 144804 ITERATIONS
SEARCH TIME: 00.00.05
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33156 ANSWERS

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L2      33156 SEA SSS FUL L1
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=ion.
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=> 12
L3      8558 L2
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=> 12 and py<1999
      8558 L2
      18916701 PY<1999
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L4 7538 L2 AND PY<1999

=> 13 and py<1999
18916701 PY<1999

L5 7538 L3 AND PY<1999

=> d hitstr 1

L5 ANSWER 1 OF 7538 CAPLUS COPYRIGHT 2003 ACS on STN

IT ***145643-18-1*** ***175071-81-5***

RL: THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(topical gels contg. N-[N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-
1-.alpha.-aspartyl]-L-phenylalanines)

RN 145643-18-1 CAPLUS

CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-
aspartyl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ structure 4 in file .gra /

RN 175071-81-5 CAPLUS

CN L-Phenylalanine, N-[5-[4-(aminoiminomethyl)phenyl]-1-oxopentyl]-L-.alpha.-
aspartyl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

/ structure 5 in file .gra /

=>
Uploading fluorinesub.str

L6 STRUCTURE UPLOADED

=> 16 sss full

FULL SEARCH INITIATED 10:04:28 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 75 TO ITERATE

100.0% PROCESSED 75 ITERATIONS
SEARCH TIME: 00.00.01

2 ANSWERS

L7 2 SEA SSS FUL L6

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE
ENTRY

TOTAL
SESSION

FULL ESTIMATED COST

148.15

303.74

FILE 'CAPLUS' ENTERED AT 10:04:51 ON 26 SEP 2003

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FILE COVERS 1907 - 26 Sep 2003 VOL 139 Iss 14
FILE LAST UPDATED: 25 Sep 2003 (20030925/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> 17

L8 1 L7

=> d hitstr 1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
IT ***149075-80-9P*** ***149075-81-0P***
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)
RN 149075-80-9 CAPLUS
CN Alanine, 3,3,3-trifluoro-N-[N-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-L-alanyl]-, methyl ester (9CI) (CA INDEX NAME)

/ structure 6 in file .gra /

RN 149075-81-0 CAPLUS
CN Alanine, 3,3,3-trifluoro-N-[N-[N-[(phenylmethoxy)carbonyl]glycyl]-L-phenylalanyl]-, methyl ester (9CI) (CA INDEX NAME)

/ structure 7 in file .gra /

=> d bib 1

L8 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2003 ACS on STN
AN 1993:496134 CAPLUS
DN 119:96134
TI Peptide modification by incorporation of .alpha.-trifluoromethyl
.alpha.-amino acids via trifluoromethyl-substituted acylimines
AU Hoess, E.; Rudolph, M.; Seymour, L.; Schierlinger, C.; Burger, K.
CS Org.-Chem. Inst., Tech. Univ. Muenchen, Garching, W-8046, Germany
SO Journal of Fluorine Chemistry (1993), 61(1-2), 163-70
CODEN: JFLCAR; ISSN: 0022-1139
DT Journal
LA English
OS CASREACT 119:96134

=> FIL STNGUIDE

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

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308.54

FILE 'STNGUIDE' ENTERED AT 10:07:00 ON 26 SEP 2003

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AND TECHNOLOGY CORPORATION, AND FACHINFORMATIONSZENTRUM KARLSRUHE

FILE CONTAINS CURRENT INFORMATION.

LAST RELOADED: Sep 19, 2003 (20030919/UP).